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Simultaneous Retrieval of Atmospheric Temperatures and Ray Paths from Occultation Spectra*

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Abstract

Simulated equivalent width data of weak lines in occultation spectra have been analyzed to retrieve both the atmospheric temperature profile and the tangent heights of the rays. It was assumed that the mixing-ratio of the absorbing gas was known but it is not necessary to know the satellite height. By analyzing lines with temperature-dependent and temperature-independent intensities temperatures accurate to 1 K and tangent heights to 0.25 km were determined over the range 20 to 90 km.

Introduction

There is considerable interest in the remote sensing of atmospheric temperature profiles. For example, temperature and pressure profiles are required to obtain vertical mixing-ratio profiles of absorbing gases from solar occultation absorption spectra.

There have been only a few attempts to obtain temperature profiles from absorption spectra. Watson and Yin (1) first proposed the use of CO_2 lines in solar spectra collected with a balloon-borne instrument. Toth (2) developed an iterative technique using the equivalent widths of high J lines of the ν_3 band of CO_2. Rinsland et al. (3) have applied the spectral-curve-fitting technique of Chang and Shaw (4) to lines of the 10.4 μm CO_2 band in solar spectra. Park et al. (5) and Park (6) have investigated the simultaneous estimation of temperature and pressures from frequency-averaged transmittance values of CO_2 near 2385 cm^{-1} and 2255 cm^{-1}.

With the exception of the methods described by Park (5,6) it has been universally assumed that all other required quantities including the height of the observing instrument and the pressure profile are known. This is not necessarily true for satellite observations and it is desirable to develop methods for retrieving information about the atmospheric paths traversed from the experimental data.

Previous investigators have noted that the sensitivity of the temperature retrieval depends on the lower state energy (E") of the line. According to Gray and Selvidge (7) the intensity S(T) of lines of linear molecules can be written

$$S(T) = S(T_o)(T_o/T)^2 \exp[1.439\ E''(T-T_o)/TT_o], \qquad (1)$$

where $S(T_o)$ is the intensity at a reference temperature T_o. The high J lines of the ν_3 CO_2 R branch, which are often proposed for temperature retrieval (2,3,5) have E" values of 1500 cm^{-1} or more. The fractional change in intensity $\Delta S/S$ per Kelvin for these lines increases monotonically from 3% at 300 K to 8% at 180 K (5). Lines with smaller lower-state energies are less temperature sensitive and have been used for pressure retrieval (5). Shaffer and Shaw (8) have suggested that these lines can be used to determine absorber amounts along a particular ray. The instrument line-of-sight can then be determined without requiring independent information of doubtful accuracy (8) provided the mixing-ratio of the absorber is known . In particular, the position of the satellite along the ray path is not required although calculations are usually carried out by assuming some arbitrary height and retrieving the corresponding set of zenith angles of the arriving rays for that position. Similarly it is assumed the latitude and hence the radius of the earth are known and the tangent height is obtained by assuming a surface pressure. The implications of these assumptions have been discussed by Shaffer et al. (8) who have shown that for earth geometries, they do not detract significantly from the accuracy.

Temperature Profile Retrieval

We have retrieved a vertical temperature profile from the simulated equivale ` widths of lines with large E" values and simultaneously obtained the apparent zenith angles of the rays which produced the spectra by including the equivalent widths of additional lines with small E".

The analysis is similar to that used by Shaffer and Shaw (9) to determine the resolution of mixing-ratio profiles. Provided a line is weak the contribution to the total equivalent width W from each layer traversed by a ray with apparent zenith angle z is additive and

$$W(z) = \rho_0 \sum_j S(T_j)\, d(T_j, A_j)\, \delta\ell_j(z), \tag{2}$$

where the mixing-ratio of the absorbing gas ρ_0 is assumed to be constant with height, $d(T_j, A_j)$ is the atmospheric density of the jth layer with temperature T_j and altitude A_j and $\delta\ell_j(z)$ is the path element through the layer.

A total of eighty equivalent widths for the four pairs of lines in Table 1 was calculated by using Eqs. (1) and (2) and dividing the U.S. Standard Atmosphere (10) from 1 to 100 km into 200 layers. For purposes of calculation the observer was at 500 km and the 40 ray paths had tangent heights spaced about 1.7 km apart between 23 and 85 km. It was assumed that useful equivalent widths for each pair of lines could be obtained over about 2 scale heights or 16 km. As indicated in Fig. 1 the ranges of tangent heights of the rays producing each pair of lines did not overlap. The line intensities were adjusted so that the largest equivalent width was the same for every line. The quantities $d(T_j, A_j)$ and $\delta\ell_j(z)$ in Eq. (2) were calculated with a computer program obtained from Snider and Goldman (11). Gaussian "noise" was added to produce simulated experimental data with a SNR of approximately 100 for the largest equivalent width values.

Because the line intensity is a nonlinear function of the temperature, an iterative technique was used to estimate the temperature profile and the zenith angles. The minimization portion of the computer program was written by

Ralston and Jennrich (12) and is available under the name BMDPAR (13). The regression analysis produces estimates of the parameters and their uncertainties by minimizing the sum of the squares of the differences between the experimental equivalent widths and those obtained from the parameter estimates.

In principle, eighty temperature and zenith angle values can be obtained by analyzing the eighty equivalent width values. However, since the uncertainty increases as the resolution increases (9) only ten temperature values were retrieved. The temperatures of the other layers in Eq. (1) were obtained by linear interpolation.

If each spectrum is taken sequentially in time and the relative times of observation are known, then the zenith angle correrponding to each spectrum can be interpolated from a small number of values, provided the zenith angle changes smoothly with time. These assumptions depend on the guiding accuracy of the optical system. In this study eleven zenith angles were retrieved and the remainder were calculated by interpolation.

Initial parameter values must be supplied in iterative analytical techniques. The ability to obtain a solution was tested by using an isothermal (240 K) atmosphere as the initial guess. The initial guesses for the zenith angles were constructed by adding a random uncertainty to the true values corresponding to an average tangent height uncertainty of about 2.5 km.

If the SNR is large and the initial parameter guesses are good a solution is obtained in a few iterations. Because of the poor initial guesses in the case described above as many as fifty iterations were necessary before the rms value of the residuals corresponded to a SNR of 100 .

Sets of simultaneously retrieved temperatures and zenith angles are given in Tables 2 and 3. These temperatures are compared with those in the Standard Atmosphere in Fig. 2. Estimated standard deviations are given in parentheses. The number of temperature parameters is the smallest which allows the principal features in the profile between 20 and 85 km to be reproduced. The differences between the "experimental" equivalent widths and those calculated from the retrieved parameters are shown in Fig. 3. These differences are essentially independent of height, indicating that a satisfactory retrieval has been obtained.

All the temperatures except those above 90 km were retrieved with an accuracy of about 1 K and the zenith angles to better than 0.005°, which corresponds to a tangent height uncertainty of about 0.25 km. It is seen from Fig. 1 that the equivalent width of each line decreases nearly exponentially with tangent height and this causes the SNR to decrease in a similar fashion. This accounts, in part, for the poor agreement between temperatures above 85 km. In addition, the accuracy of the estimates is reduced by the lack of equivalent widths corresponding to rays above 85 km.

It was found that the correlations between the retrieved values of the zenith angles and the temperatures were small. This is due to the very different dependences of the absorber amounts along the paths with tangent height and the change of temperature with height in the atmosphere. However, the retrieved tangent heights of the rays do depend on the temperature profile. If the temperature profile is assumed to be known then only the tangent heights of the rays have to be retrieved. The effects of assuming a ten parameter temperature profile with incorrect values for the temperature parameter at 33 km on the retrieved tangent heights are shown in Fig. 4. The greatest error occurs near 33 km. These results indicate that accurate temperature profiles are required if accurate ray paths are to be determined.

Other retrievals have been made by estimating temperatures at equally spaced height intervals of 10 km. As expected, the temperature profile is not reproduced as well as in Fig. 2 but the differences can be attributed to the poor model used.

Conclusions

It has been shown that the temperature profile and ray paths can be simultaneously estimated from the simulated equivalent widths of weak absorption lines of a gas whose mixing-ratio is known. The estimates depend on the characteristics of the spectra available for analysis including the number of lines, their intensities and lower state energies and the model used for the temperature profile. The results described here were obtained with a minimal number of lines. Although it has been assumed that the mixing-ratio of the absorber is constant with height, as for example CO_2, N_2 or O_2, it is only necessary that the mixing-ratio be known.

References

1. J. R. G. Watson and P. K. L. Yin, "Possibility of atmospheric temperature sounding by the solar occultation technique," Appl. Opt. 14, 549 (1975).
2. R. A. Toth, "Temperature sounding from the absorption spectrum of CO_2 at 4.3 μm," Appl. Opt. 16, 2661 (1977).
3. C. P. Rinsland et al., "Stratospheric Temperature Profile From Balloon-Borne Measurements of the 10.4 μm Band of CO_2," J. Quant. Spectrosc. Radiat. Transfer, 30, 327 (1983).
4. Y. S. Chang et al., "Determination of Abundances of Gases from Solar Spectra," J. Quant. Spectrosc. Radiat. Transfer, 19, 599 (1978).
5. J. H. Park et al., "Solar occultation sounding of pressure and temperature using narrowband radiometers," Appl. Opt., 19, 3132 (1980).
6. J. H. Park, "Effect of interoferogram smearing on atmospheric limb sounding by Fourier transform spectroscopy," Appl. Opt., 21, 1356 (1982).
7. C. D. Gray and J. E. Selvidge, "Relative Intensity Calculations for Carbon Dioxide," J. Quant. Spectrosc. Radiat. Transfer, 5, 291 (1965).
8. W. A. Shaffer, J. H. Shaw and C. B. Farmer, "Effects of systematic errors on the mixing-ratios of trace gases obtained from occultation spectra," Appl. Opt. (in press).
9. W. A. Shaffer and J. H. Shaw, "Resolution of vertical mixing ratio profiles of atmospheric constituents retrieved from solar spectra," Appl. Opt. 22, 2977 (1983).
10. U. S. Standard Atmosphere, 1976 (U.S. GPO, Washington, D.C., 1976).
11. D. E. Snider and A. Goldman, "Refractive Effects in Remote Sensing of the

Atmosphere with Infrared Transmission Spectroscopy," BRL Report 1790, Ball. Res. Lab., Aberdeen Proving Grounds Md. (1975).

12. M. L. Ralston and R. I. Jennrich, "DUD, a Derivative-free Algorithm for Non-Linear Least Squares," Technometrics, <u>20</u>, 7 (1978).

13. "BMDP-1982," in Biomedical Computer Programs, P Series, M. Brown ed. (U. California Press, Berkeley, 1982).

TABLE 1

Intensities and lower state energies of line pairs used and the tangent height range for each pair.

Line Pair	Line Intensity (296 K) $[cm^{-1}/mol\ cm^{-2}]$	$E''[cm^{-1}]$	Tangent Height Range [km]
1	7.2×10^{-22} 3.5×10^{-23}	2000 0	22 → 38
2	2.3×10^{-21} 5.3×10^{-22}	2000 0	40 → 54
3	2.3×10^{-20} 3.7×10^{-21}	2000 0	56 → 70
4	1.2×10^{-18} 2.3×10^{-20}	2000 0	71 → 85

TABLE 2

Retrieved Temperatures (K) Compared with Corresponding Values of the U.S. Standard Atmospheres Temperature Profile

Altitude (km)	Temperature			
	Initial Guess	Retrieved T_R	Standard Atmosphere T_C	Difference $(T_R - T_C)$
100	240	245(280)	195.1	50.6
95	240	150(20)	188.4	-38.4
86	240	186.8(1.3)	186.9	-0.1
70	240	218.0(4)	219.6	-1.6
60	240	247.5(4)	247.0	+0.5
51	240	271.5(9)	270.6	+0.9
48	240	271.8(6)	270.6	+1.2
40	240	250.3(4)	250.4	-0.1
33	240	230.1(4)	231.0	-0.9
20	240	216.2(6)	216.6	-0.4

TABLE 3

The eleven estimated zenith angles used to model the 40 ray paths of the simulated data.

Zenith Angles (Degrees)				Tangent Heights (km)
Initial Guess	Retrieved z_R	Correct z_C	Difference $(z_R - z_C)$	
109.95	109.984(14)	110.000	-0.016	85
110.196	110.153(4)	110.149	-0.004	79
110.241	110.299(2)	110.299	0.000	73
110.387	110.448(2)	110.448	0.000	67
110.532	110.597(1)	110.597	0.000	60
110.778	110.747(2)	110.747	0.000	[illegible]4
110.786	110.893(2)	110.896	-0.003	48
111.069	111.047(1)	111.045	+0.002	42
111.115	111.200(3)	111.195	+0.005	35
111.360	111.342(1)	111.344	-0.002	29
111.506	111.495(1)	111.493	+0.002	24

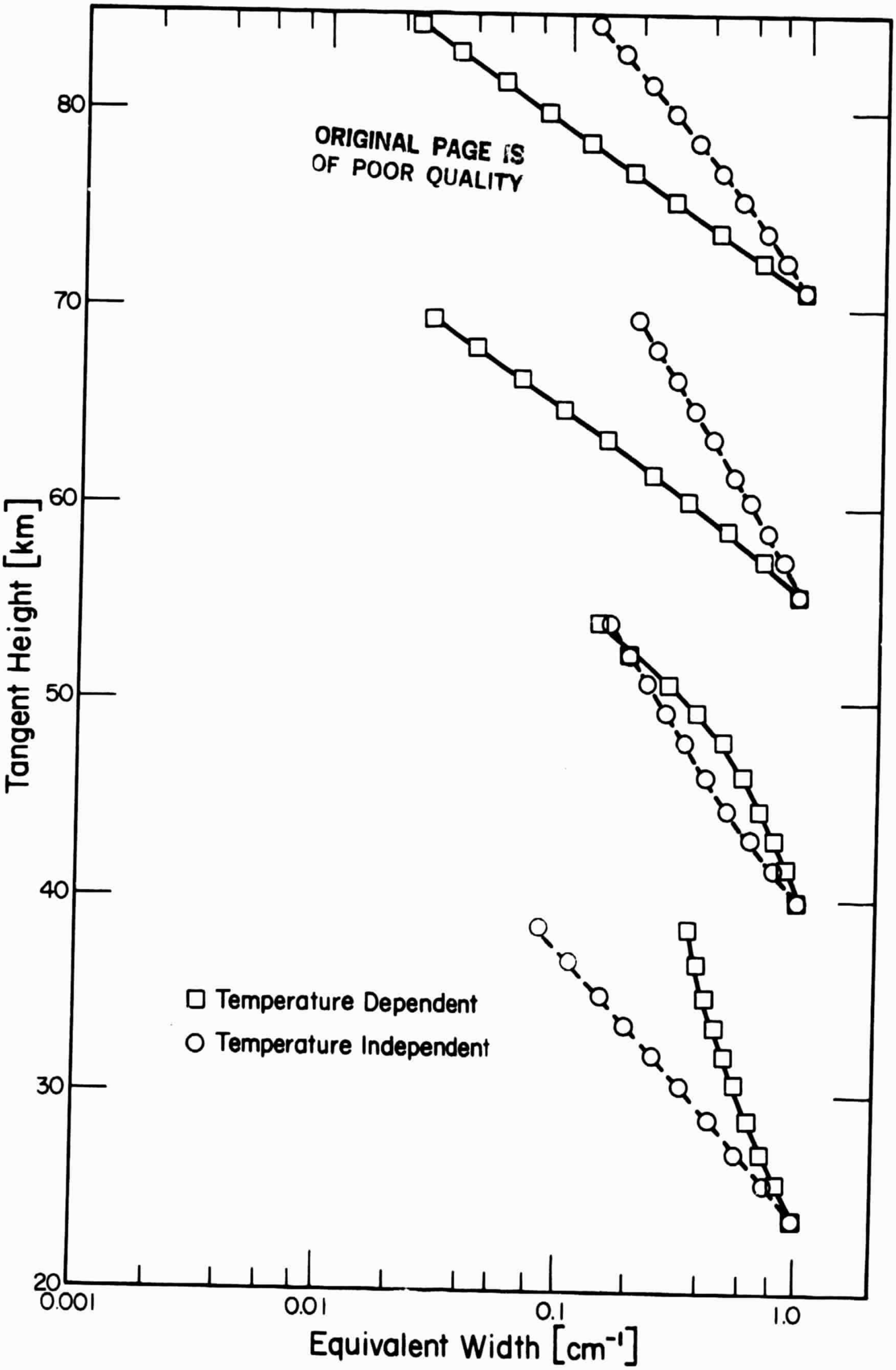
Figure Captions

FIG. 1 The simulated equivalent width data calculated from Eqs. 1 and 2 using the line parameters in Table 1 and the U.S Standard Atmosphere.

FIG 2 A. U.S. Standard Atmosphere temperature profile, showing initial 240 K guess of the temperature profile. B. Differences between U.S. Standard Atmosphere Temperature profile and temperature calculated from parameter estimates in Table 2.

FIG 3 Residuals between the estimated widths W_e calculated using the U.S. Standard Atmosphere Temperature profile and correct ray paths and the widths W_c calculated using the retrieved temperature and zenith angle parameters in Table 2 and 3.

FIG 4 Changes in the zenith angle retrieved with the model temperature profile fixed, including a systematic error ΔT in the parameter of altitude 33 km.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Tangent Height [km]
80
70
60
50
40
30
20
0.001
0.01
0.1
1.0
Equivalent Width [cm⁻¹]
Temperature Dependent
Temperature Independent

Fi's. 1

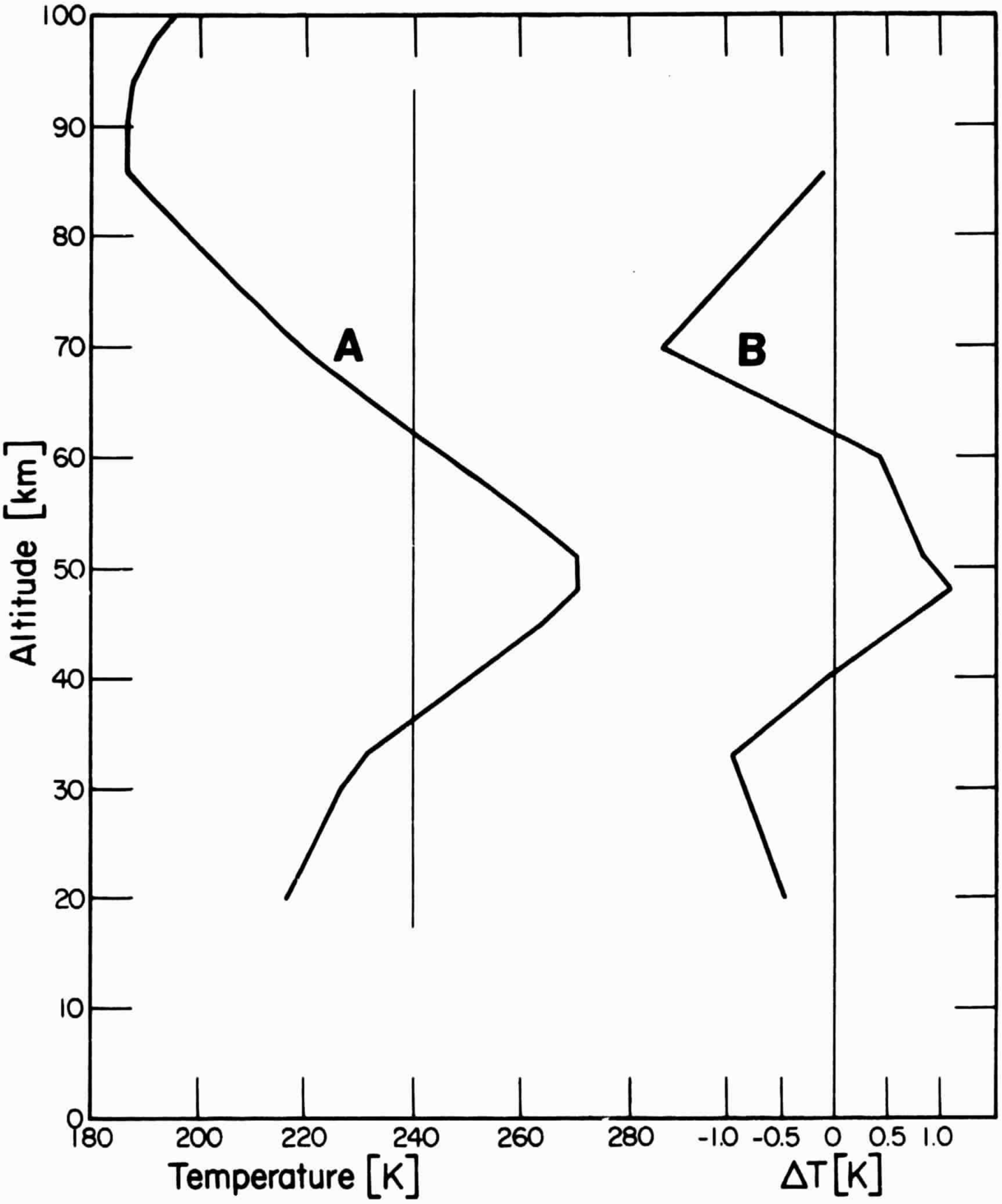
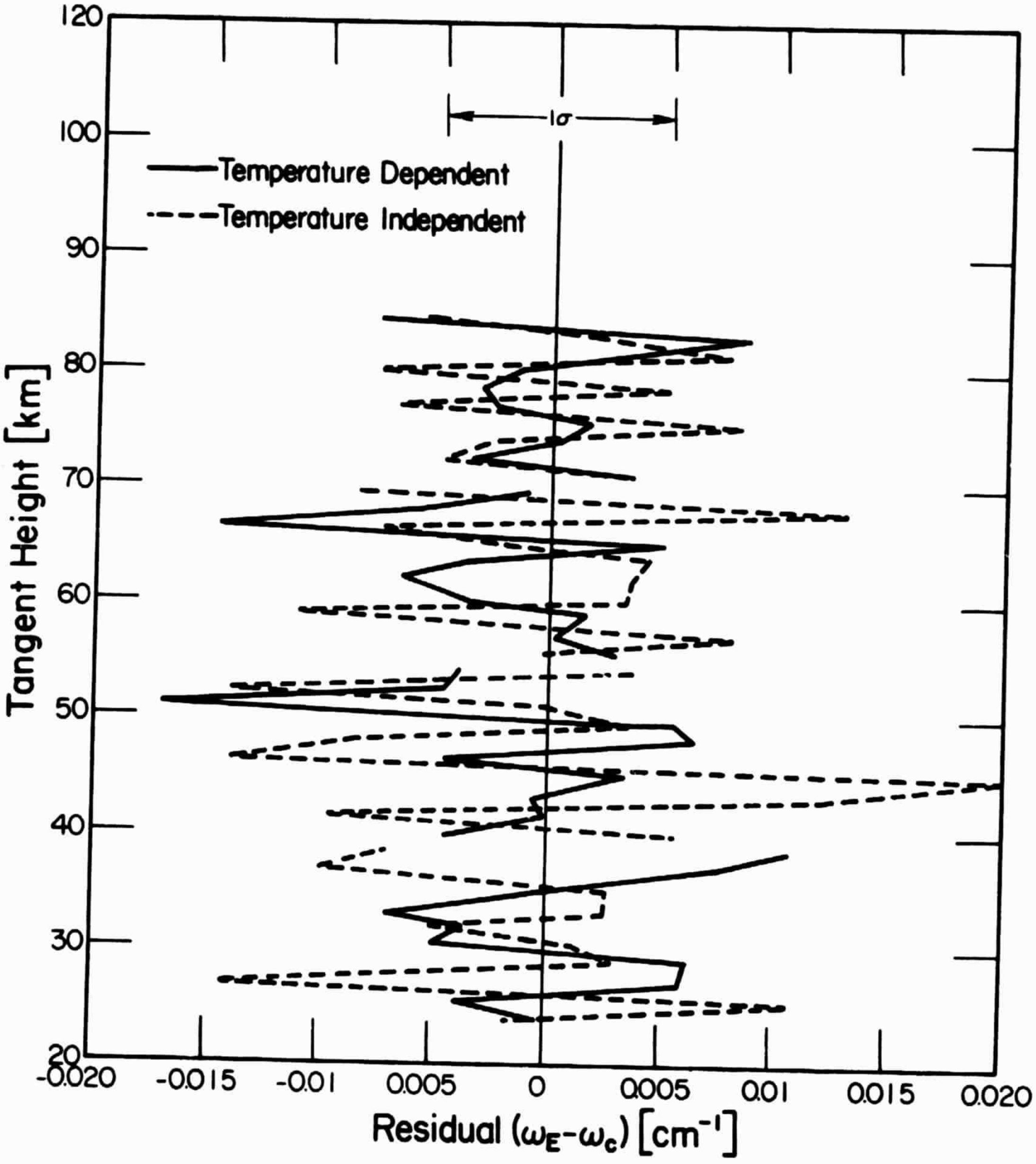

100
90
80
70
60
50
40
30
20
10
0
Altitude [km]
A
B
180
200
220
240
260
280
-1.0
-0.5
0
0.5
1.0
Temperature [K]
ΔT [K]

Fig. 2


120
100
90
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70
60
50
40
30
20
1σ
Temperature Dependent
Temperature Independent
Tangent Height [km]
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-0.015
-0.01
0.005
0
0.005
0.01
0.015
0.020
Residual (ω_E-ω_c) [cm^{-1}]

Fig. 3

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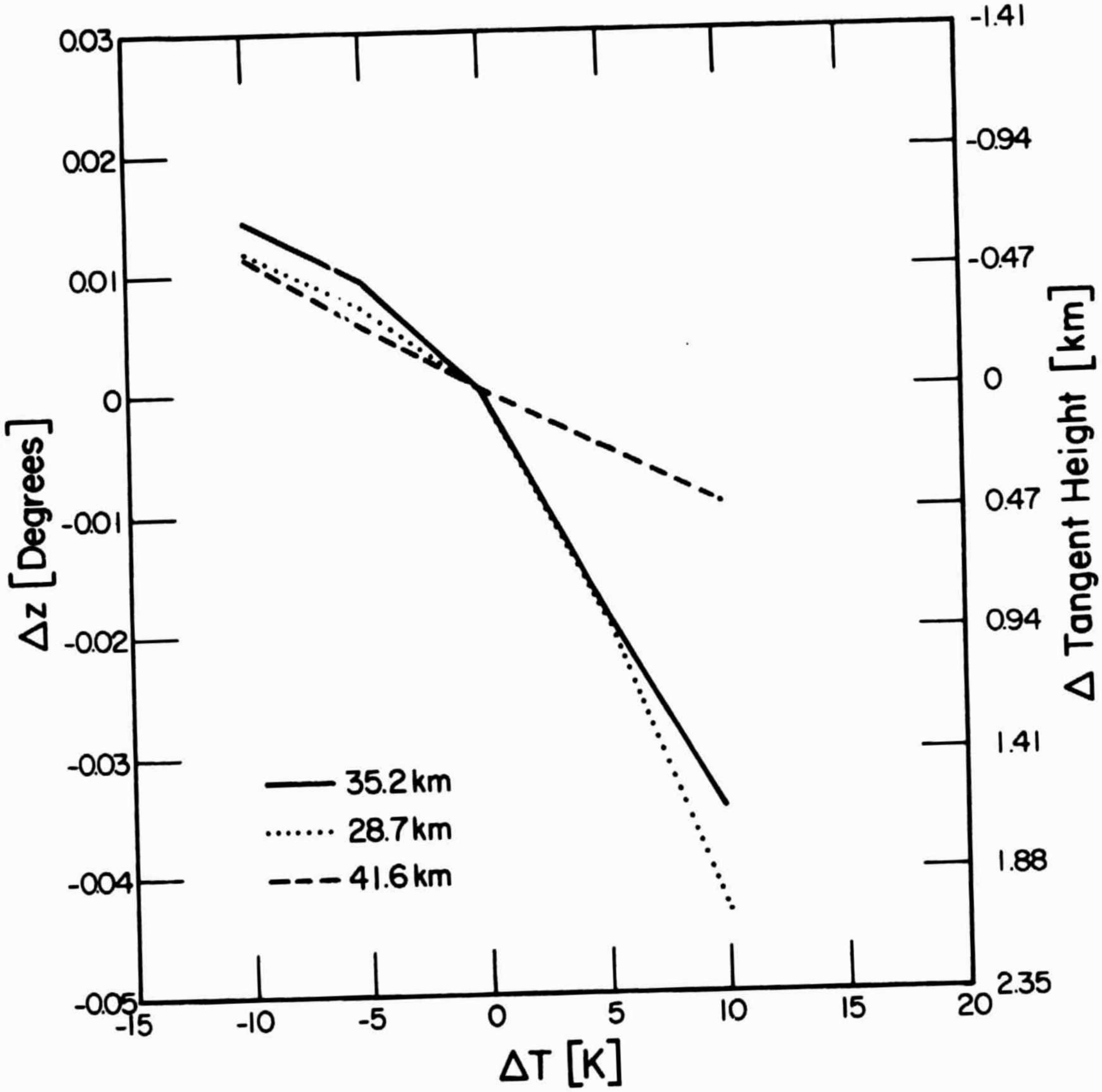

Fig. 4